Abstract No. jian523
P097 - A Hypothetical Yeast Protein
J.-S. Jiang, N. Manning, and H. Kycia (BNL, Biology)
Beamline(s): X12C, X25

Introduction: P097 is a yeast protein (YNL200C) from a DNA fragment of the yeast chromosome XIV. It consists of 246 amino acids with a molecular weight 27.5 kDA. P097 was one of selected gene targets in structural genomics (http://proteome.bnl.gov). P097 was targeted for structure determination because it is a member of a large protein family (23 sequences currently represented in ProDom - domain PD005835) with unknown biological function.

Methods and Materials: A three-wavelength seleno-methionine MAD data were collected at beam line X12C (Table 1). Reflections were observed with diffraction up to 1.90 Angstroms. Data were processed by DENZO/SCALEPACK. The initial structure was solved within two hours by using Automated Structure Determination Platform - ASDP (http://asdp.bnl.gov) after completing MAD data collection.

Results: The final model of P097 structure revealed a three-layer $\alpha-\beta-\alpha$ sandwich (Figure 1), with two molecules forming a tightly packed dimer (Figure 2). The red spherical balls represent putative metal ions that were observed in the electron density map. Each monomer consists of 8 β-strands and 9 α-helices. The topology of P097 suggests a likely NAD(P)-binding Rossmann fold, which features at least 6 β-strands in a row, with the first and the sixth strand following an alpha helix. A multiple alignment of similar sequences with at least 30% identity to P097 revealed a couple of conserved regions. The putative metal ions are around by the conserved residues in a protein/solvent pocket where may indicate an important substrate binding site. The biological function of P097 as related to structural genomics is under further investigation.

Table 1. Summary of MAD data collection at X12C/NSLS and statistics for P097

Space group	P212121
Unit cell parameters	a=57.75Å, b=68.64Å, c=125.21Å, α=β=γ=90.0°.
Specimen to detector	89.9mm
Rotation increment	1.0 degree per image
Number of images	360 per data set
Exposure time	30 seconds per image

	Peak	Inflection	Remote
Wavelength (Å)	0.9785	0.9788	0.9400
Resolution range (Å)	50-1.9 (1.97-1.90)	50-1.9 (1.97-1.90)	50-1.9 (1.97-1.90)
Reflections	39403	39416	39366
R-merge	0.063 (0.390)	0.062 (0.446)	0.062 (0.417)
Completeness	98.3% (88.2%)	98.5% (90.8%)	98.2% (92.3%)
I/sigma > 20	44.7% (2.2%)	45.1% (2.1%)	45.2% (5.4%)
Redundancy > 12	41.6%	41.5%	44.1%

Figure 1. P097 monomer is a three-layer $\alpha-\beta-\alpha$ sandwich. The topology of P097 suggests a likely NAD(P)-binding Rossmann fold. β strands are painted as cyan, α helices are painted as red and loops are painted as grey
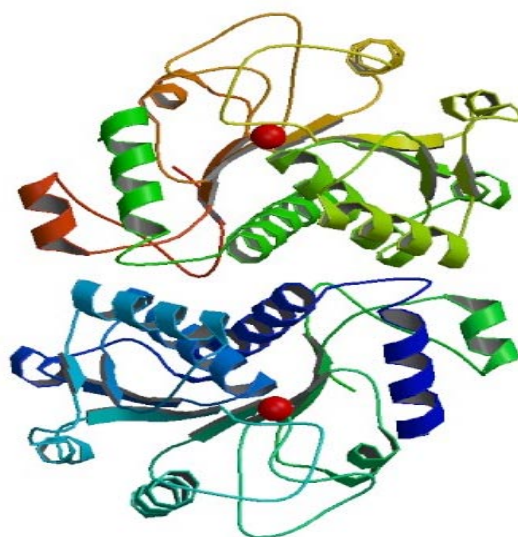
Figure 2. P097 forms a tightly packed dimer. Large red spheres represent putative metal ions.